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Third Annual Report

Report Period: September 1, 1968 to December 31, 1969

An Investigation of Near Critical and Super-Critical
Burning of Fuel Droplets

by

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Abstract

This report summarizes the work done under NASA contract NGR 39-009-077 for the period September 1, 1968 to December 31, 1969. Principle accomplishments of the report period are briefly discussed and publications arising from the research are listed. Experimental droplet burning rates were obtained at atmospheric pressure in a combustion gas environment. Burning rates were measured for n-paraffins and alcohols at gas temperatures in the range 1650-2550°K and oxygen concentrations in the range 0-40%. The use of the diffusion flame theories of droplet combustion, both constant and variable property, gave burning rate predictions within 40% of the measurements over the test range. However, the theories showed a systematic failure with increasing fuel molecular weight. Theoretical and experimental work was also done at high pressures to investigate droplet combustion in the critical region. Allowance for real gas effects and ambient gas solubility in the liquid phase had a substantial effect in determining the pressures required for a supercritical combustion. The value of the Lewis number also exerts a strong influence on the pressure requirements for supercritical combustion, with the pressure increasing for lower Lewis numbers.

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I. Introduction

This third annual report is a summary of the principle accomplishments made under NASA Contract No. NGR-39-009-077 during the period September 1, 1968 to December 31, 1969. The findings of this research are presented in more detail in the several technical reports and papers published during the present report period.^{1,2,3,4} The results of the program have technical application in the design of liquid-fueled rocket engine combustion chambers.

The computation of droplet life histories has become a basic step in the design of combustion chambers for liquid fueled rocket engines.⁵ The overall objective of this investigation is to study the evaporation and combustion of droplets in order to further develop computational techniques for estimating droplet life histories and transient evaporation under rocket engine combustion chamber conditions. Particular emphasis is on combustion at elevated pressures where the influence of the droplet approaching its critical point must be considered.

The work of this report period has been divided into two phases. In the first phase, droplet evaporation and combustion was studied in the combustion products of a flat flame burner, in order to simulate the thermal environment of a rocket engine combustion chamber. This work was conducted at atmospheric pressure for ambient gas temperatures in the range 1650-2550°K and ambient oxygen concentrations in the range 0-40% for various

normal paraffin and alcohol droplets. The results of the experiments were compared with various theoretical methods, in order to establish accurate computational procedures for droplet life history calculations.

The second phase of the study considered droplet evaporation and combustion at high pressures. Wieber,⁶ has computed the total pressures required for supercritical evaporation of oxygen and n-heptane droplets in a high temperature inert environment. This analysis was based on a quasisteady, constant property treatment of the gas phase, neglecting ambient gas solubility and other high pressure corrections in the determination of equilibrium conditions at the droplet surface. In the present study, these calculations have been extended to investigate high pressure combustion of various hydrocarbon droplets.

Manrique⁷ and Savery⁸ have shown that high pressure corrections and ambient gas solubility are significant factors in liquid-vapor equilibrium near the critical point. A variable property, quasisteady analysis, which includes ambient gas solubility, has been developed to examine these high pressure effects for both evaporation and burning droplets. The theoretical results have been compared with experiments conducted in a zero-gravity apparatus, described in Ref. (1).

II. Flat Flame Study

The experimental arrangement for this study consisted of a flat flame burner mounted on rails so that it could be quickly moved under a test droplet and brought to a stop.^{3,4} The rapid immersion of the droplet in the hot gases leaving the burner provided a good simulation of a droplet entering a combustion chamber. Measurements were made of the time variation of droplet diameter and temperature for comparison with theoretical predictions.

The burner was operated at atmospheric pressure, with various mixtures of carbon monoxide, hydrogen, oxygen and nitrogen in order to obtain a variety of temperatures (1650-2550°K) and oxygen concentrations (0-40% by volume) in the ambient gas around the droplet. The composition and temperature of the gas surrounding the droplet were determined from thermochemical calculations allowing for dissociation and heat loss to the burner. In order to obtain a broad range of fluid properties, normal paraffins ranging from pentane to hexadecane, and alcohols from methyl to decyl alcohol were tested.

The experimental results were compared with predictions from various droplet evaporation and combustion theories.^{9,10} Over the entire range of testing the simplified, constant property diffusion flame theories gave reasonable agreement with the experimental results, with maximum errors on the order of 40% for droplet burning rates. Comparison between the constant

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property solution and a variable property solution due to Goldsmith and Penner,¹⁰ was quite good, with errors on the order of 6%.

All the theoretical models were found to progressively overestimate the burning rate of the fuel with increasing fuel molecular weight. This failure was attributed to fuel decomposition in the region between the droplet surface and the oxidation zone.

Flame luminousity was observed very early in the heat-up period of the droplet (on the order of 10 to 20% of the heat-up time). Motivated by this experimental finding, the steady droplet burning theories were extended to allow the computation of droplet heat and mass transfer rates during heat-up. Using this theory, droplet life histories were computed and compared with the experimental results. The errors in the computed life histories were about the same as those encountered for steady burning rates. The extended model gave a reasonably good prediction of the influence of combustion on the droplet heat-up time.

III. High Pressure Study

The theoretical study of high pressure droplet combustion began with the use of the extended, constant property droplet heat-up analysis described in the previous section. The calculations also considered droplet evaporation without combustion for comparison with Wieber's⁶ calculations.

The results were found to be quite sensitive to the value of the Lewis number. For Lewis numbers greater than or near unity, the computations indicated that supercritical burning would occur for pressures near the critical pressure. With decreasing Lewis number, the pressure required for supercritical combustion progressively increased. For burning droplets, the ambient oxygen concentration did not exert a strong influence on the pressures required for supercritical burning in the range air-pure oxygen.

The present calculations for n-heptane evaporation were not in good agreement with Wieber's results. For example, in the absence of convection, Wieber finds that supercritical burning will occur when the pressure is about 2.4 times the critical pressure for n-heptane. For the same situation, the present results indicated supercritical burning at 1.5 times the critical pressure. This was found to be a Lewis number effect resulting from differences in the assumed value of fuel thermal conductivity (the value employed in Wieber's calculations appears to be low in comparison to values given in the literature, Ref.12).

The experimental results indicated that the pressures required for supercritical burning were, somewhat fortuitously, more on the order of Wieber's prediction. Real gas effects were examined next as a possible cause of the discrepancy between the present theory and the experimental results. This involved a consideration of variable fluid properties in the gas phase, as well as high pressure corrections in the determination of liquid-vapor equilibrium at the droplet surface.

The variable property gas phase analysis was an extension of the Goldsmith and Penner¹⁰ analysis which included simultaneous evaporation of dissolved gas along with the fuel. Particular emphasis was placed on determining droplet conditions during steady burning, as well as the pressure levels required for supercritical combustion.

Several models of increasing complexity were employed to compute equilibrium conditions at the droplet surface. The simplest model corresponded to the case where all high pressure corrections are neglected. This corresponds to the earlier constant property work and shows the influence of the variable property gas phase analysis.

In the other models, high pressure corrections were considered through the use of a modified Redlich-Kwong equation of state with mixing rules given by Prausnitz.¹¹ The first of these considered high pressure and temperature droplet evaporation in a single inert gas (carbon dioxide or nitrogen). Finally, a more tentative

solution was investigated for a burning droplet which considers the solubility of hydrocarbon combustion products (carbon dioxide, water, nitrogen) in the droplet liquid.

A parametric study for the simplest model (no high pressure corrections) indicated that combustion temperature was not a very sensitive parameter, values from 2000 to 4000°K causing less than a 10% change in the reduced total pressure required for supercritical burning (P_{RCB}). Once again the solution was more sensitive to the Lewis number, a $\pm 20\%$ variation yielding a $\pm 15\%$ change in P_{RCB} .

For the evaporation of n-heptane, P_{RCB} was found to be 1.25, compared to 1.5 for the earlier constant property solution and 2.4 from Ref. (6). Thus, consideration of variable gas phase properties does not provide an explanation of the disagreement between theory and experiment.

The calculations indicated that water would condense on the droplet during steady burning for all paraffins lighter than n-pentane, invalidating the gas phase analysis for these materials. For heavier hydrocarbons, regions were found where water would condense during the heat-up period.

Allowing for high pressure effects causes an increase in the computed value of P_{RCB} for evaporation in carbon dioxide and nitrogen. For example, with n-decane droplets evaporating in carbon dioxide, $P_{RCB} = 1.75$ for the corrected solution, compared to 1.35 for the uncorrected solution. For pressure ratios greater than P_{RCB} , the droplet reaches the supercritical evaporation condition at liquid temperatures below the critical temperature of the pure fuel. Rather

large quantities of the ambient gas are dissolved in the liquid phase near the critical mixing point, e.g. 38% CO₂ concentration for n-decane at a total pressure three times the critical pressure of pure n-decane. At a fixed total pressure, there is a complicated variation of ambient gas solubility with increasing temperature (increasing in some regions and decreasing in others). This effect will also introduce complications in the analysis of droplet heat-up at high pressures.

For the case of hydrocarbon combustion, the solubility of water, carbon dioxide and nitrogen (for combustion in air) must be considered. This results in a quaternary liquid mixture, which when coupled with the difficulties in accurately treating the thermodynamics of water (which is polar), increases the uncertainty of the results. However, consideration of this case does yield P_{RCB} in the range 2.0-2.5 for n-decane combustion, which is in general agreement with the experimental results.

Experimental measurements of supercritical combustion conditions were made using the apparatus and procedures of Ref. (1). Droplets were ignited in a pressurized chamber under zero-gravity conditions and measurements were made of the liquid temperature during the lifetime of the droplet. A supercritical burning condition was assumed when the droplet temperature rose continuously, following ignition, with no sign of leveling out at a steady burning state.

The most recent measurements with this apparatus have employed several improvements over the earlier work reported in Ref. (1).

This has involved using smaller thermocouples (.001 inch O.D.) and shielding the lead wires from the flame, with small quartz tubes, in order to reduce conduction errors. The experiments have considered n-octane and n-decane droplets in various oxygen-nitrogen mixtures ranging from air to pure oxygen.

IV Future Work

The use of the flat flame burner apparatus is continuing at atmospheric pressure. One new series of tests involves a study of hydrazine, MMH UDMH droplet combustion under both decomposition and oxidation conditions.

A second series of tests with the atmospheric pressure flat flame burner is examining the influence of convection on bipropellant droplet combustion at high ambient temperatures. In these experiments, a porous sphere is used to simulate a droplet. This technique provides a larger range of Reynolds number than is currently possible with supported droplets.

A pressurized version of the flat flame burner apparatus is under development to study high pressure droplet evaporation and combustion in a combustion gas environment. This apparatus will also employ the porous sphere technique to simulate a droplet.

Work is also continuing on the theory of high pressure droplet combustion. The Benedict - Webb - Rubin equation of state, modified for mixtures,¹³ is being employed to compute equilibrium conditions at the droplet surface. The results of these calculations will be compared with the present theoretical results, which employs the Redlich-Kwong equation of state, in order to examine the influence of the equation of state on the results. Further experimental results in this area will involve the determination of droplet temperatures at steady burning and pressures required for supercritical burning for n-tridecane and n-hexadecane.

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